COMPONENTS:	EVALUATOR:
(1) p-Xylene; C <sub>8</sub> H <sub>10</sub> ; [106-42-3] (2) Water; H <sub>2</sub> O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	January 1986.

### CRITICAL EVALUATION:

Quantitative solubility data for the p-xylene (1) - water (2) system have been reported in the publications listed in Table 1.

Reference	T/K	Solubility	Method
Andrews and Keefer (ref 1)	298	(1) in (2)	spectrophotometric
Bohon and Claussen (ref 2)	274-316	(1) in (2)	spectrophotometric
Pryor and Jentoft (ref 3)	316-577	(1) in (2)	synthetic
Guseva and Parnov (ref 4)	414-531	(1) in (2)	unspecified
Hoegfeldt and Bolander (ref 5)	298	(2) in (1)	Karl Fischer
Polak and Lu (ref 6)	273,298	mutual	GLC, Karl Fischer
Sutton and Calder (ref 7)	298	(1) in (2)	GLC
Kirchnerova and Cave (ref 8)	298	(2) in (1)	Karl Fischer
Price (ref 9)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 10)	298	(1) in (2)	GLC
Sanemasa <i>et al</i> . (ref 11)	288-318	(1) in (2)	spectrophotometric

The original data in all these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into three parts.

# 1. SOLUBILITY OF p-XYLENE (1) IN WATER (2)

All the available data on the solubility of p-xylene in water are summarized in Table 2 with the exception of the high temperature data of Pryor and Jentoft (ref 3) and Guseva and Parnov (ref 4) which are discussed in the next section. The 298K datum of Krzyzanowska and Szeliga (ref 10) has also been excluded from consideration because it does not appear to have been obtained independently of that of Price (ref 9).

The various data for p-xylene in water (Table 2) are in only fair agreement and none of the averaged values are Recommended. At 298K the values cluster around two values: 0.019 (ref 1, 2, 6) and 0.016 g(1)/100g sln (ref 6, 7, 9, 11). Although the values of Bohon and Claussen (ref 2) in well characterized systems are often high this is not sufficient justification for favouring the lower values (ref 7, 9, 11) at this stage. At other temperatures,

(continued next page)

- (1) p-Xylene;  $C_8H_{10}$ ; [106-42-3]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### **EVALUATOR:**

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

January 1986.

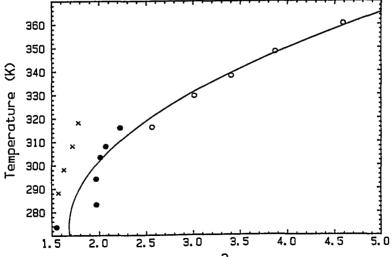
CRITICAL EVALUATION: (continued)

TABLE 2: Tentative Values of the Solubility of p-Xylene (1) in Water (2)

T/K	Solubility values			
	Reported values $^a$	"Best" value	s (± o <sub>n</sub> )	
	10 <sup>2</sup> g(1)/100g sln	10 <sup>2</sup> g(1)/100g sln	10 <sup>5</sup> x <sub>1</sub>	
273	1.55° (ref 2), 1.64 (ref 6)	1.60 ± 0.05	2.7	
283	1.97 (ref 2)	2.0	3.4	
293	1.96* (ref 2), 1.60* (ref 11)	1.8 ± 0.2	3.1	
298	2.00 (ref 1), 1.98 (ref 2), 1.85 (ref 6), 1.56 (ref 7), 1.57 (ref 9), 1.63 (ref 11)	1.8 ± 0.2	3.1	
303	2.02* (ref 2), 1.68 (ref 11)	1.9 ± 0.2	3.2	
313	2.20* (ref 2), 2.5* (ref 3), 1.75 (ref 11)	2.2 ± 0.3	3.7	
323	2.8* (ref 3)	2.8	4.7	
333	3.2* (ref 3)	3.2	5.4	
343	3.6* (ref 3)	3.6	6.1	
353	4.2* (ref 3)	4.2	7.1	
363	4.8* (ref 3)	4.8	8.1	

a Values marked with an asterisk (\*) have been obtained by the Evaluator by graphical interpolation of the original data.

c Refers to solubility of solid.



Solubility (10<sup>2</sup>g(1)/100g sln)

FIGURE 1. Solubility of p-xylene in water; selected data: ref 2 (•), ref 3 (o); ref 11 (x). Solid line drawn through "Best" values (Table 2). (continued next page)

b Obtained by averaging where appropriate;  $\sigma_{\mathbf{n}}$  has no statistical significance.

COMPONENTS:	EVALUATOR:
(1) p-Xylene; C <sub>8</sub> H <sub>10</sub> ; [106-42-3] (2) Water; H <sub>2</sub> O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

CRITICAL EVALUATION: (continued)

agreement is equally poor and at higher temperatures (323-363K) only the values of Pryor and Jentoft (ref 3) are available. Clearly this system warrants further investigation. Selected data have been plotted in Figure 1 which emphasizes the differences among the available data.

Thermodynamic functions derived from various data sets by application of the van't Hoff equation are summarized in Table 3.

TABLE 3: Thermodynamic Functions for the Dissolution of p-Xylene in Water Derived from Solubility Data

Reference	$^{\Delta \mathrm{H}_{ exttt{sln}}}$ kJ mol $^{-1}$	ΔC <sub>p,sln</sub> <sub>J K-l mol-l</sub>
Bohon and Claussen (ref 2)	3.9	-211
Pryor and Jentoft (ref 3)	$7.8^{\alpha}_{b}$ 30.4	122 <sup>a</sup> 81 <sup>b</sup>
Guseva and Parnov (ref 4)	16.0	210
Sanemasa <i>et al</i> . (ref 11)	3.2	11
"Best" values (Table 2)	6.9	204

a 316 < T < 360 K b 434 < T < 568 L

Comparison of the thermodynamic data in Table 3 with similar but better characterized hydrocarbon systems (e.g. benzene in water) suggests that none of the solubility data for p-xylene in water are very reliable (including the "Best" values).

2. SOLUBILITY OF p-XYLENE (1) IN WATER (2) AT ELEVATED TEMPERATURES

Solubility data for p-xylene in water at elevated temperatures (ca. 400-570K) and system pressure in sealed tubes have been reported by Pryor and Jentoft (ref 3) and Guseva and Parnov (ref 4). The results are plotted in Figure 2 and are clearly in poor agreement. In the absence of confirmatory data it is not possible to know which set is more reasonable. Thermodynamic functions derived from both data sets (Table 3) are in poor agreement and differ markedly from low T values. The interested user is referred to the relevant Data Sheets for the experimental values.

(continued next page)

- (1) p-xylene;  $C_8H_{10}$ ; [106-42-3]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### **EVALUATOR:**

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

January 1986.

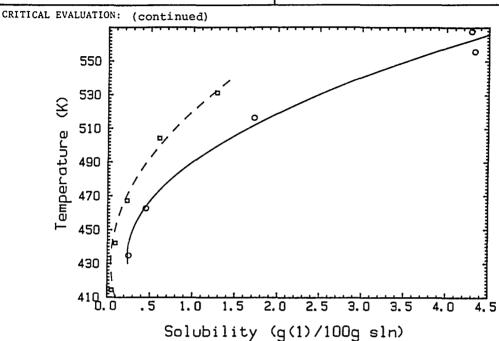


FIGURE 2. Solubility of p-xylene in water at elevated temperatures: ref 3 (o); ref 4 ( $\square$ ).

# 3. THE SOLUBILITY OF WATER (2) IN p-XYLENE (1)

The solubility of water in p-xylene has been determined only at 298K. All the available data are collected in Table 4. The results are in excellent agreement and the mean is Recommended.

TABLE 4: Recommended (R) Value of the Solubility of Water (2) in p-Xylene (1)

T/K	Solubili	ty values	
	Reported values $10^2 { m g}(2)/100 { m g}$ sln	"Best" value ( $\pm \sigma$ $10^2$ g(2)/100g sln 1	
298	4.5 (ref 5), 4.40 (ref 6), 4.57 (ref 8)	4.5 ± 0.1 (R) 2	.6 (R)

a Obtained by averaging;  $\sigma_{f n}$  has no statistical significance.

- Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. 1949, 71, 3644-7.
- 2. Bohon, R.L.; Claussen, W.F. J. Am. Chem. Soc. 1951, 73, 1571-8.
- 3. Pryor, W.A.; Jentoft, R.E. *J. Chem. Eng. Data* <u>1961</u>, 6, 36-7. (continued next page)

- (1) p-Xylene;  $C_8H_{10}$ ; [106-42-3]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### **EVALUATOR:**

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

January 1986

CRITICAL EVALUATION: (continued)

### REFERENCES (continued)

- 4. Guseva, A.N.: Parnov, E.I. Vestn. Mosk. Univ. Khim. 1963, 18, 76-9.
- 5. Hoegfeldt, E.; Bolander, B. Ark. Kemi <u>1964</u>, 21, 161-86.
- 6. Polak, J.; Lu, B.C.-Y. Can. J. Chem. 1973, 51, 4018-23.
- 7. Sutton, C.; Calder, J.A. J. Chem. Eng. Data 1975, 20, 320-2.
- 8. Kirchnerova, J.; Cave, G.C.B. Can. J. Chem. 1976, 54, 3909-16.
- Price, L.C. Am. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44; see also Ph.D. Dissertation 1974, University of California, Riverside, CA, U.S.A., 1973, quoted in ref 22.
- Krzyzanowska, T.; Szeliga, J. Nafta (Katowice) 1978, 34, 413-7.
- Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. 1982, 55, 1054-62.

### **ACKNOWLEDGEMENT**

The Evaluator thanks Dr Brian Clare for the regression analyses and graphics.

# COMPONENTS: (1) p-Xylene; C<sub>8</sub>H<sub>10</sub>; [106-42-3] Andrews, L.J.; Keefer, R.M. (2) Water; H<sub>2</sub>O; [7732-18-5] J. Am. Chem. Soc. 1949, 71, 3644-77. VARIABLES: One temperature: 25°C PREPARED BY: A. Maczynski and Z. Maczynska

### EXPERIMENTAL VALUES:

The solubility of p-Xylene in water at  $25^{\circ}$ C was reported to be 0.0200 g(1)/100 g sln.

The corresponding mole fraction,  $x_1$ , calculated by the compilers is  $3.39 \times 10^{-5}$ .

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25 C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

### SOURCE AND PURITY OF MATERIALS:

- (1) Eastman Kodak Co. best grade; fractionally distilled; b.p. 138.5 C.
- (2) Not specified.

ESTIMATED ERROR:

Not specified.

- (1) p-Xylene; C<sub>8</sub>H<sub>10</sub>; [106-42-3]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Bohon, R.L.; Claussen, W.F.

J. Am. Chem . Soc. 1951, 73, 1571-8.

### VARTABLES .

PREPARED BY:

Temperature: 0.4-42.8°C

G.T. Hefter

### EXPERIMENTAL VALUES:

### Solubility of p-xylene in water

t/°C	g(1)/100g sln <sup>a</sup> (compiler)	$10^{5}x_{1}$ (compiler)
0.4	0.0156 <sup>b</sup>	2.64 <sup>b</sup>
10.0	$0.0188^{b}$	$3.19^b$
10.0	0.0197	3.34
14.9	0.0195	3.31
21.0	0.0197	3.34
25.0	0.0198 <sup>c</sup>	3.36°
25.6	0.0199	3.37
30.2	0.0201	3.41
30.3	0.0204	3.46
34.9	0.0207	3.51
35.2	0.0207	3.51
42.8	0.0222	3.76

<sup>&</sup>lt;sup>a</sup> Solubilities of (1) in (2) were reported as "optical density" (absorbance) measurements. Solubilities were calculated by the compiler using the Beer-Lambert law, the stated cell path-length (1 cm) and the authors' "extinction coefficients" (absorptivities) and corrected optical densities. This gave a solubility of g(1)/L sln which was then converted to g(1)/100g sln by assuming a solution density of 1.00 kg/L.

## AUXILIARY INFORMATION

### METHOD /APPARATUS / PROCEDURE:

A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24h and then allowed to settle for at least another 24h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tared, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a quartz cuvette and measured in a Beckman DU spectrophotometer. Absorbances were corrected for adsorption of (1) onto the walls of the cuvette.

### SOURCE AND PURITY OF MATERIALS:

- (1) Eastman Kodak Co., purified by recrystallization from ethanol, washing, filtering through silica gel then distilling. Purity was determined by refractometry (no details given).
- (2) Air-free conductivity water, no other details given.

### ESTIMATED ERROR:

Temp. ± 0.02°C

Soly. ± 0.5% relative

 $<sup>^</sup>b$ Data refer to solubility solid (1) in (2).

 $<sup>^</sup>c$  Given in the original paper as 0.198g(1)/L sln.

- (1) p-Xylene;  $C_8H_{10}$ ; [106-42-3]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Pryor, W.A.; Jentoft, R.E.

J. Chem. Eng. Data 1961, 6, 36-7.

### VARIABLES:

Temperature: 43.0-294.5°

### PREPARED BY:

A. Maczynski and Z. Maczynska

### EXPERIMENTAL VALUES:

### Solubility of p-xylene in water

Cloud point	t/°C Cloud point	Midpoint	$10^{3}x_{1}$	q(1)/100 q sln
appears	disappears			(compiler)
42.8	43.3	43.0	0.0434	0.0256
54.4	58.3	56.4	0.0510	0.0301
61.7	68.3	65.0	0.0576	0.0340
73.9	76.7	75.3	0.0656	0.0387
85.0	89.4	87.2	0.0779	0.0459
161.7	163.3	162.5	0.4264	0.2508
186.7	189.5	188.1	0.7686	0.4514
241.6	244.9	243.2	2.9555	1.7174
280.5	284.4	282.5	7.6238	4.3326
291.6	298.3	294.5	7.5407	4.2871

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Mixture of (1) and (2) were carefully weighed into glass ampoules. The ampoules were sealed allowing just enough space for thermal expansion. The ampoule, observed through a telescope from behind a safety barrier, was suspended in a 4-liter stirred silicone oil bath, and the bath was heated until the (1) dissolved. On cooling, a cloud of fine (1) droplets appeared, making the suspension opaque. The temperature was raised until the cloud dis-The cycle was repeated appeared. three to four times until reliable appearance and disappearance temperatures for the cloud were recorded.

### SOURCE AND PURITY OF MATERIALS:

- (1) source not specified; 99.1% by freezing point; main impurities are isomeric xylenes; used as received.
- (2) not specified.

### ESTIMATED ERROR:

not specified.

# COMPONENTS: ORIGINAL MEASUREMENTS: (1) p-Xylene; C<sub>8</sub>H<sub>10</sub>; [106-42-3] Guseva, A.N.; Parnov, E.I. (2) Water; H<sub>2</sub>O; [7732-18-5] Vestn. Mosk. Univ. Khim. 1963, 18, 76-9. VARIABLES: PREPARED BY: Temperature: 141 - 258°C A. Maczynski and Z. Maczynska

### EXPERIMENTAL VALUES:

Solubility of p-xylene in water

t/°C	g(1)/100 g sln	10 <sup>4</sup> x <sub>1</sub> (compiler)	
141	0.049	0.83	
169	0.096	1.63	
194	0.231	3.93	
231	0.607	10.34	
258	1.283	22.00	

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: (1) source not specified; The measurements were made in sealed glass tubes. No details $n_D^{20}$ 1.4958. were reported in the paper. (2) doubly distilled. ESTIMATED ERROR: not specified. REFERENCES:

- (1) p-Xylene;  $C_8H_{10}$ ; [106-42-3]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Hoegfeldt, E.; Bolander, B.

Ark. Kemi, 1964, 21, 161-86.

### VARIABLES:

One temperature: 25°C

### PREPARED BY:

A. Maczynski and Z. Maczynska

### EXPERIMENTAL VALUES:

The solubility of water in p-Xylene was reported to 0.022 mol(2)  $L^{-1}$  sln.

The corresponding mass percent and mol fraction,  $x_2$ , calculated by the compilers are 0.045 g(2)/100 g sln and 0.0027.

The assumption that 1.00 L sln = 857 g sln was used in the calculation.

### AUXILIARY INFORMATION

## METHOD/APPARATUS/PROCEDURE:

The water determination was carried out according to Johansson's modification of the Karl Fischer titration described in ref 1, 2.

# SOURCE AND PURITY OF MATERIALS:

- (1) Fluka; 0.04% of ethylbenzene; purity 99.8%; used as received.
- (2) Not specified.

### ESTIMATED ERROR:

Temp. ±0.3°C

Soly. ±0.002 mol(2) L<sup>-1</sup> sln (type of error not specified)

- Hardy, C.J.; Greenfield, B.F.; Scargill, D. J. Chem. Soc. 1961, 90.
- Johansson, A.
   Sv. Papperstidn. 1947, 11B, 124.

# COMPONENTS: ORIGINAL MEASUREMENTS: (1) p-Xylene; C<sub>8</sub>H<sub>10</sub>; [106-42-3] Polak, J.; Lu, B.C.-Y. (2) Water; H<sub>2</sub>O; [7732-18-5] Can. J. Chem. 1973, 51, 4018-23. VARIABLES: PREPARED BY: Temperature: 0-25°C A. Maczynski and Z. Maczynska

### EXPERIMENTAL VALUES:

### Solubility of p-xylene in water

t/°C	mg(1)/kg(2)	g(1)/100 g sln (compiler)	10 <sup>5</sup> x <sub>1</sub> (compiler)
0†(a)	164(c)	0.0164	2.78
25 (b)	185 (c)	0.0185	3.14

The solubility of water in p-xylene at 25°C was reported to be 440 mg(1)/kg(2).

The corresponding mass percent and mole fraction,  $x_2$ , calculated by the compilers are 0.0440 g(2)/100 g sln and  $2.59 \times 10^{-3}$ .

a-c See "Estimated Error" †p-xylene was at supercooled liquid state.

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Approximately 50 mL of (1) together with (2) were placed in a 125 mL Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr and left in the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis.

The solubility of water in the organic layer was determined by Karl Fischer titration and the solubility of hydrocarbon in the water layer was determined by gas chromatography.

### SOURCE AND PURITY OF MATERIALS:

- (1) Eastman Organics, pure grade reagent; shaken three times with distilled water.
- (2) distilled.

# ESTIMATED ERROR:

temp. (a)  $\pm$  0.02°C, (b)  $\pm$  0.01°C soly. (c)  $\pm$  1.7% (from two or three determinations)

- (1) p-Xylene;  $C_8H_{10}$ ; [106-42-3]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Kirchnerova, J.; Cave, G.C.B.

Can. J. Chem. 1974, 54, 3909-16.

### VARIABLES:

One temperature: 25°C

### PREPARED BY:

A. Maczynski and Z. Maczynska

### EXPERIMENTAL VALUES:

The solubility of water in p-xylene at 25°C was reported to be 0.0217 mol(2)/L and  $x_2 = 0.00269$ . The corresponding mass percent calculated by the compilers is 0.0457 g(2)/100 g sln.

### AUXILIARY INFORMATION

## METHOD/APPARATUS/PROCEDURE:

Approximately 50 mL of (1) was placed in the equilibration vessel. A test tube containing 6 mL of (2) was then placed in the vessel so that the rim of the test tube rested against the upper inside wall of the vessel. The vessel was then stoppered, placed inside a plastic bag, and the jacketed vessel was emersed up to its neck in a water thermostat. Trials had shown that the stoichiometric concentration of (1) in (2) became constant within 2 days. The stoichiometric concentration of water was determined by a conventional Karl Fischer dead-stop back-titration.

# SOURCE AND PURITY OF MATERIALS:

- (1) Fisher 277; purified by double crystallization.
- (2) not specified.

# ESTIMATED ERROR:

temp. ± 0.1°C soly. 0.0002 mol(2) dm<sup>-3</sup> sln (standard deviation from 5 determinations).

- (1) p-Xylene; C<sub>8</sub>H<sub>10</sub>; [106-42-3]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Sutton, C.; Calder, J.A.

J. Chem. Eng. Data 1975, 20, 320-2.

# VARIABLES:

One temperature: 25°C

### PREPARED BY:

A. Maczynski and Z. Maczynska

### EXPERIMENTAL VALUES:

The solubility of p-xylene in water at 25°C was reported to be 156.0 mg(1)/kg(2). The corresponding mass percent and mole fraction,  $x_1$ , calculated by the compilers are 0.01560 g(1)/100 g sln and  $2.65 \times 10^{-5}$ .

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The concentration of (1) in (2) was determined by gas chromatography.

# SOURCE AND PURITY OF MATERIALS:

- (1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.
- (2) distilled.

### ESTIMATED ERROR:

temp. ± 0.1°C soly. 1.6 mg(1)/kg(2) (the standard deviation of the mean for six replicates)

- (1) p-Xylene;  $C_{8}H_{10}$ ; [106-42-3]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Price, L.C.

Am. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44.

### VARIABLES:

One temperature: 25°C

### PREPARED BY:

M.C. Haulait-Pirson

### EXPERIMENTAL VALUES:

The solubility of p-xylene in water at 25°C and at system pressure was reported to be 157.0 mg(1)/kg(2). The corresponding mass percent and mole fraction,  $x_1$ , calculated by the compiler are 0.0157 g(1)/100 g sln and 2.66 x  $10^{-5}$ .

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GSC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

# SOURCE AND PURITY OF MATERIALS:

- (1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.
- (2) distilled.

### ESTIMATED ERROR:

temp. ± 1°C

 $soly. \pm 1.0 mg(1)/kg(2)$ 

- (1) p-Xylene;  $C_8H_{10}$ ; [106-42-3]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Krzyzanowska, T.; Szeliga, J.

Nafta (Katowice), 1978, 12, 413-7.

### **VARIABLES:**

One temperature: 25°C

### PREPARED BY:

M.C. Haulait-Pirson

### EXPERIMENTAL VALUES:

The solubility of p-xylene in water at  $25^{\circ}$ C was reported to be 157.0 mg(1)/kg(2).

The corresponding mass percent and mole fraction,  $x_1$ , calculated by compiler are 0.0157 g(1)/100 g sln and 2.66 x  $10^{-5}$ .

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page).

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150-mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.

### SOURCE AND PURITY OF MATERIALS:

- (1) not specified.
- (2) not specified.

### ESTIMATED ERROR:

soly. 3.9 mg(1)/kg(2) (standard
deviation from 7-9 determinations).

- (1) p-Xylene;  $C_8H_{10}$ ; [106-42-3]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H.

Bull. Chem. Soc. Jpn. 1982, 55, 1054-62.

### VARIABLES:

PREPARED BY:

Temperature: 15-45°C

G.T. Hefter

### EXPERIMENTAL VALUES:

The solubility of p-xylene in water

t/°C	$10^3 \text{ mol(1)/dm}^3 \text{ sln}$	g(1)/100 g sln (compiler) <sup>a</sup>	$10^5 x_1$ (compiler) $\alpha$
15	1.48	0.0157	2.67
25	$1.53 \pm 0.07$	0.0163	2.76
35	1.61 ± 0.08	0.0172	2.92
45	1.66 ± 0.05	0.0178	3.02

- a Assuming solution densities to be the same as those of pure water at the same temperature (ref 1).
- b No error given.

# AUXILIARY INFORMATION

### METHOD /APPARATUS / PROCEDURE:

The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm³ of (2) and 10-20 cm³ of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was established a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm³ aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.

# SOURCE AND PURITY OF MATERIALS:

- (1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 98.0%, used without further purification.
- (2) Redistilled; no further details given.

# ESTIMATED ERROR:

soly. see table, type of error not specified. temp. ± 0.1°C.

- Kell, G.S.
   J. Chem. Eng. Data <u>1975</u>, 20, 97.
- Sanemasa, I.; Araki, M.;
   Deguchi, Y.; Nagai, H.
   Chem. Lett. 1981, 225-8.

- (1) p-Xylene;  $C_8H_{10}$ ; [106-42-3]
- (2) Artificial seawater (ref 1)

### ORIGINAL MEASUREMENTS:

Sutton, C.; Calder, J.A.

J. Chem. Eng. Data 1975, 20, 320-2.

### **VARIABLES:**

One temperature: 25.0°C

One salinity: 34.5 g salts/kg sln

### PREPARED BY:

M. Kleinschmidt

### EXPERIMENTAL VALUES:

The solubility of p-xylene in artificial seawater is reported to be 110.9 mg(1)/kg sln. The corresponding mass percent and mole fraction,  $x_1$  calculated by the compiler are 0.01109 g(1)/100 g sln and 1.93 x  $10^{-5}$  assuming the artificial seawater composition of ref 1.

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

### SOURCE AND PURITY OF MATERIALS:

- (1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure.
- (2) made from doubly distilled water and salts 99+% pure.

# ESTIMATED ERROR:

temp. ± 0.1°C

soly. 0.9 (std. dev.)

### REFERENCES:

Lyman, J.; Fleming, R.H.;
 J. Mar. Res. <u>1940</u>, 3, 135.